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KINETIC MODELING OF GAS MIXTURES

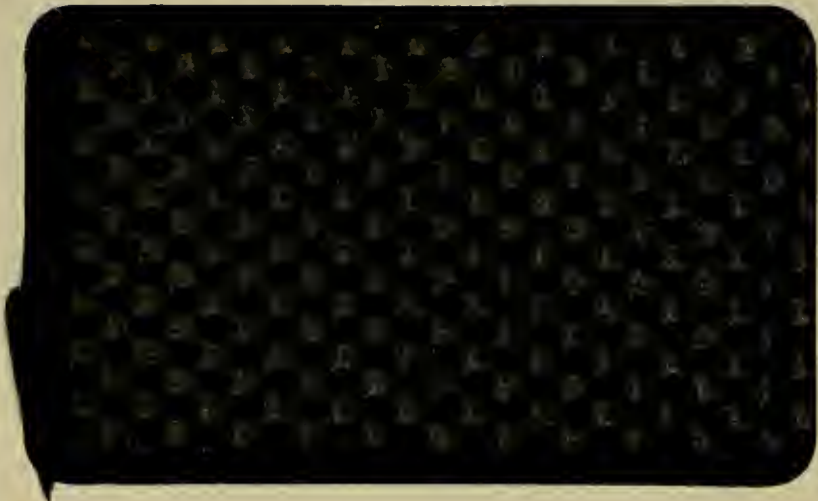
Lawrence Sirovich

1 February 1962

AEC Research and Development Report

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ABSTRACT

Kinetic models for multi-component gases are given. It is shown that some of the most important features of the Boltzmann equation are retained in spite of the simplicity of the model equations. An iteration procedure on the model equation is carried out and is identified with the Chapman-Enskog procedure. Linear and non-linear formal procedures for developing the models and their extensions are also given

Table of Contents

	Page
Abstract	2
Section	
1. Introduction	4
2. Background and Notation	5
3. Model Equations	10
4. Transport Theory	14
Appendices	
A. Formal Derivation of the Binary Model Equations and Higher Approximations -- Linear Theory	21
B. Maxwell Force Modeling	30
C. Non-Linear, Non-Maxwell Modeling	33
D. Collision Integral Approximations	37

KINETIC MODELING OF GAS MIXTURES

1. Introduction

In the well-known paper of Bhatnager, Gross, and Krook¹ a simplified kinetic equation is exhibited.² It in essence approximates the Boltzmann collision operator by a drastically simpler expression which nonetheless still retains some of the gross features of the exact Boltzmann equation. In this note a generalization of this model to gas mixtures is given.³ A special case of these equations was developed together with R. Liboff in the Spring of 1960. They were subsequently applied by him in an extensive treatment of wave propagation in a plasma.⁴

For reasons of exposition some of the more important results will be relegated to a series of appendices at the end of this note. After a short section, mainly devoted to notation, we postulate the model equations and briefly exhibit some essential features, notable those given by the relaxation theory. Following

1. P. L. Bhatnager, E. P. Gross, and M. Krook, Phys. Rev. 94, 511 (1954).
2. The same kinetic model was postulated independently by P. Welander, Arkiv för Fysik 7, 507 (1954).
3. Although the work of reference 1 applies to a binary plasma, the treatment is essentially for a single component. For in this treatment one species exists as a Maxwellian background.
4. R. Liboff, "Propagation of Long Wavelength Disturbances in a Plasma", NYO-9762, Courant Institute of Mathematical Sciences, New York University (1961).

this we give a type of a Chapman-Enskog procedure for these equations. This, of course, reveals a great deal about the nature of the model equations. The appendices, among other things, give linear and non-linear formal procedures for developing the model equations and further extensions of them.

Although we speak of gas mixtures, nothing more complicated than a binary gas is considered in detail. We are given this license because a binary gas already contains all the complexity of an n-component gas since collisions themselves are binary. In this way we are relieved of the notational burden imposed by a multicomponent analysis. Also in this connection we introduce in the next section a simplified notation which avoids much of the ubiquitous subscripts found in the subject, but which cannot be easily used for more than a two-component gas.

2. Background and Notation

We consider a binary gas made up of what we shall call an upper case (U.C.) gas and a lower case (L. C.) gas, with the following notation:

(U.C.)	Quantity	(L.C.)
F	number density in phase space	f
U	streaming velocity	u
T	temperature	τ
N	number density in configuration space	n
k	Boltzmann's constant	k
M	mass	m
$R = k/M$	gas constant	$r = k/m$
$F_o = \frac{N}{(2\pi RT)^{3/2}} e^{-\frac{(\xi-U)^2}{2RT}} \quad \text{Maxwellian} \quad f_o = \frac{n}{(2\pi r\tau)^{3/2}} e^{-\frac{(\xi-u)^2}{2r\tau}}$		

ξ refers to the molecular velocity. As usual⁵

$$(2.1) \quad \int F \begin{bmatrix} 1 \\ \xi \\ M \frac{(\xi-U)^2}{2} \end{bmatrix} d\xi = \begin{bmatrix} N \\ NU \\ 3/2 NkT \end{bmatrix}$$

and similarly for the lower case gas. In addition to the two Maxwellians defined above, we shall also require

$$(2.2) \quad \tilde{F}_o = \frac{N}{(2\pi RT)^{3/2}} e^{-\frac{(\xi-\tilde{u})^2}{2RT}}$$

5. Some authors define a partial temperature, i.e., a temperature associated with the mean energy of a species relative to the mean velocity of the entire gas.

and

$$(2.3) \quad \tilde{f}_o = \frac{n}{(2\pi rT)^{3/2}} e^{-\frac{(\xi - \tilde{u})^2}{2r\tilde{T}}}$$

where \tilde{u} is the mass averaged velocity

$$(2.4) \quad \tilde{u} = \frac{MNU + mnu}{mn + MN}$$

and \tilde{T} is the mean temperature of the binary gas

$$(2.5) \quad \frac{3}{2} k\tilde{T} = \frac{e}{\tilde{n}} = \frac{\int (MF + mf) \tilde{c}^2 / 2 d\xi}{\int (F + f) d\xi}.$$

We have denoted the relative molecular velocity by \tilde{c} ,

$$(2.6) \quad \tilde{c} = (\xi - \tilde{u})$$

and it will also be convenient to define

$$(2.7) \quad c = (\xi - U)$$

and

$$(2.8) \quad c = (\xi - u).$$

We write the Boltzmann equations of the binary gas as

$$(2.9) \quad \left(\frac{\partial}{\partial t} + \xi \cdot \frac{\partial}{\partial x} + \mathcal{F} \cdot \frac{\partial}{\partial \xi} \right) F = J_{FF} + J_{Ff}$$

$$(2.10) \quad \left(\frac{\partial}{\partial t} + \xi \cdot \frac{\partial}{\partial x} + f \cdot \frac{\partial}{\partial \xi} \right) f = J_{ff} + J_{fF} .$$

Here \mathcal{F} denotes the force per unit mass on the (U.C.) gas and f the force per unit mass on the (L.C.) gas. For simplicity we take these to be velocity independent. The collision terms will not be specified, and one is referred to the standard source by Chapman and Cowling.⁶ J_{FF} refers to the self collision of the (U.C.) gas and J_{Ff} to the cross collisions, and similarly for the (L.C.) gas. Denoting by

$$(2.11) \quad J(\phi) = \int \phi J \, d\xi$$

we have the following invariants of molecular collisions,

$$(2.12) \quad J_{ff}(1, \xi, \xi^2) = J_{FF}(1, \xi, \xi^2) = 0$$

$$(2.13) \quad J_{fF}(m\xi, m\xi^2) + J_{FF}(M\xi, M\xi^2) = 0 .$$

For details see for instance the article by H. Grad.⁷ Using these relations one may easily derive the so-called conservation equations,^{6,7} given as follows

6. S. Chapman and T. G. Cowling, The Mathematical Theory of a Non-Uniform Gas, Cambridge Univ. Press (1952).

7. H. Grad, "Theory of Rarefied Gases", in Rarefied Gas Dynamics, F. Devienne, ed., Pergamon Press (London, 1960).

Continuity

$$(2.14) \quad \left\{ \begin{array}{l} \frac{\partial N}{\partial t} + \frac{\partial}{\partial x} \cdot (NU) = 0 \\ \frac{\partial n}{\partial t} + \frac{\partial}{\partial x} \cdot (nu) = 0 \\ \frac{\partial \tilde{\rho}}{\partial t} + \frac{\partial}{\partial x} \cdot (\tilde{\rho}\tilde{u}) = 0 \end{array} \right.$$

with total mass density

$$(2.15) \quad \tilde{\rho} = MN + mn .$$

Momentum

$$(2.16) \quad \tilde{\rho} \frac{\partial \tilde{u}}{\partial t} + \rho \tilde{u} \cdot \frac{\partial}{\partial x} \tilde{u} + \frac{\partial}{\partial x_i} \cdot \tilde{P}_{ij} = MN \mathcal{F} + mn \mathcal{f}$$

with stress

$$(2.17) \quad \tilde{P}_{ij} = \int (mf + MF) \tilde{c}_i \tilde{c}_j d\xi .$$

Energy

$$(2.18) \quad \begin{aligned} \frac{\partial}{\partial t} \tilde{e} + \frac{\partial}{\partial x} \cdot (\tilde{e}\tilde{u}) + \frac{\partial}{\partial x_i} \cdot \tilde{Q}_i + \tilde{P}_{ij} \frac{\partial \tilde{u}_i}{\partial x_j} \\ = MN \mathcal{F} (U - \tilde{u}) + mn \mathcal{f} (u - \tilde{u}) \end{aligned}$$

with heat flow

$$(2.19) \quad Q_i = \int [mf + MF] \frac{\tilde{c}_i}{2} \tilde{c}^2 d\xi .$$

We shall frequently make use of the following conversion relations, which are easily verified,

$$(2.20) \quad (U-\tilde{u}) = mn/\tilde{\rho} \ (U-u)$$

$$(2.21) \quad (u-\tilde{u}) = MN/\tilde{\rho} \ (u-U)$$

$$(2.22) \quad \tilde{n}k(\tilde{T}-T) = nk(\tau-T) + \frac{MN \ mn}{3\tilde{\rho}} (U-u)^2$$

$$(2.23) \quad \tilde{n}k(\tilde{T}-\tau) = Nk(T-\tau) + \frac{MN \ mn}{3\tilde{\rho}} (U-u)^2 \ .$$

Note that (2.20,21) may be used in (2.18) to give a more symmetric form. A word of caution is appropriate at this point. Frequently in what follows, deviations from the mean are replaced by relative differences by means of (2.20-23); this, however, can be carried out only for a two-component gas.

3. Model Equations

It has been pointed out in the literature⁷ that the temporal evolution of a two-component gas, up until the hydrodynamic stage, may roughly be described as occurring in three epochs. First the component of lighter mass experiences equilibration, then the other species undergoes equilibration, and finally the entire gas

experiences equilibration. This sequence of events has more or less formed the basis for the set of equations which are now postulated. In Appendices A, B, C, various formal procedures are given for obtaining these equations.

For the (U.C.) gas,

$$(3.1) \quad \left(\frac{\partial}{\partial t} + \xi \cdot \frac{\partial}{\partial x} + \mathcal{J} \cdot \frac{\partial}{\partial \xi} \right) F = \Gamma (F_O - F) - \frac{\mu_{F_O}^F}{NkT} (U-u) \cdot C \\ - \frac{3v_{F_O}}{2kNT} \left(\frac{C^2}{2RT} - 1 \right) (T-\tau) + \frac{\mu_{M_O}^F}{NkT} (U-u)^2 \left(\frac{C^2}{2RT} - 1 \right),$$

$$(3.2) \quad \left(\frac{\partial}{\partial t} + \xi \cdot \frac{\partial}{\partial x} + \mathcal{J} \cdot \frac{\partial}{\partial \xi} \right) f = \gamma (f_O - f) - \frac{\mu_{f_O}^f}{nk\tau} (u-U) \cdot c \\ - \frac{3vf_O}{2nk\tau} \left(\frac{c^2}{2r\tau} - 1 \right) (\tau-T) + \frac{\mu_{m_O}^f}{nk\tau} (U-u)^2 \left(\frac{c^2}{2r\tau} - 1 \right)$$

where

$$(3.3) \quad \mu_M = \frac{\mu_{Mn}mn}{\tilde{\rho}} \left[\frac{1}{MN} - \frac{\varepsilon(n-N)}{nM(m+M)} \right]$$

and

$$(3.4) \quad \mu_m = \frac{\mu_{MN}mn}{\rho} \left[\frac{1}{mn} - \frac{\varepsilon(N-n)}{nN(m+M)} \right].$$

One notices that the first term of the right hand side of (3.1) and (3.2) is that found in models of a simple gas.^{1,2} This represents the self-collisions of a gas species. The remaining three terms involve the velocity and temperature differences of the two gases, and represent the cross-collisions of the two

gases. The generalization to a multi-component gas is clear. One merely attaches subscripts to the velocities and temperatures and replaces the last three terms by three summations of these quantities over all species.

The quantities Γ , γ , μ , ν , ε are positive and at most functions of density and temperature, and we will say something of their choice in the next section. The complicated forms given by (3.3,4) are not really necessary, but are what are suggested by an exact theory given for Maxwell molecules in Appendix B. Expressions for μ , ν , and ε in the latter case are given in that appendix. A short calculation shows that, independent of the choice of Γ , γ , μ , ν , and ε , equations (3.1) and (3.2) preserve the collisional invariants (2.12,13). This, of course, guarantees the conservation equations of the last section. To indicate the equilibration behavior of the mixture, we consider the relaxation theory of the set (3.1,2). For simplicity we disregard the forces \mathcal{F} and f , and take γ , Γ , μ , ν , ε to be constants. Our equations are now,

$$(3.5) \quad \frac{\partial}{\partial t} F = \Gamma (F_o - F) - \frac{\mu F_o}{NkT} (U-u) \cdot C - \frac{\nu F_o}{NkT} \left(\frac{C^2}{3RT} - 1 \right) (T-\tau) \\ + \mu_M \frac{F_o}{NkT} (U-u)^2 \left(\frac{C^2}{3RT} - 1 \right) ,$$

$$(3.6) \quad \frac{\partial}{\partial t} f = \gamma (f_o - f) - \frac{\mu f_o}{nk\tau} (u-U) \cdot c - \frac{\nu f_o}{nk\tau} \left(\frac{c^2}{3r\tau} - 1 \right) (\tau-T) \\ + \mu_m \frac{f_o}{nk\tau} (U-u)^2 \left(\frac{c^2}{3r\tau} - 1 \right) .$$

It is an immediate consequence of the conservation equations of the last section that n , N , \tilde{u} , \tilde{T} are constants. On taking velocity and temperature moments of equations (3.5) and (3.6) we get by routine calculations,

$$(3.7) \quad \frac{\partial}{\partial t} (U-u) = -\mu \left(\frac{1}{MN} + \frac{1}{mn} \right) (U-u)$$

$$(3.8) \quad \frac{\partial}{\partial t} (T-\tau) = -\frac{\nu}{k} \left(\frac{1}{N} + \frac{1}{n} \right) (T-\tau) + \frac{2}{3k} \left(\frac{\mu_M}{N} - \frac{\mu_m}{n} \right) (U-u)^2.$$

Such a simple system is easily solved and since we took μ and ν to be positive, the velocity and temperature differences of the two species vanish exponentially in time. And by an earlier remark they approach the mean gas properties. Further, we can easily compute the equations for all higher moments such as stress, heat conduction, etc., for each gas. We then find that all higher moments (higher than density, temperature and velocity) have a relaxation time of $1/\bar{\Gamma}$ for the (U.C.) gas and a relaxation time of $1/\gamma$ for the (L.C.) gas. We thus see that the (U.C.) and (L.C.) gases become locally Maxwellian in times $O(1/\bar{\Gamma})$, $O(1/\gamma)$ respectively, and that they relax to each other in a time proportional to $\max[O(1/\nu), O(1/\mu)]$. In order to obtain the sequence of events mentioned at the outset of this section we need only adjust the magnitudes of $(\mu, \nu, \gamma, \bar{\Gamma})$.

4. Transport Theory

As an indication of the scope of the theory covered by equations (3.1), (3.2), we develop some of the related transport properties. Our main goal will be to gain a comparison with the results of the Chapman-Enskog procedure. Instead of a successive approximation technique we will find it more convenient to use an iteration procedure.⁸

Denoting the differential operator of (3.1,2) by D , we employ the following iteration procedure,

$$(4.1) \quad DF^{(p)} = \left[(F_0 - F^{(p+1)}) - \mu \frac{F_0 (U-u) \cdot C}{NkT} \right. \\ \left. - \frac{3vF_0}{2NkT} \left(\frac{C^2}{2RT} - 1 \right) (T-\tau) + \frac{\mu_M F_0}{NkT} (U-u)^2 \left(\frac{C^2}{3RT} - 1 \right) \right]$$

and the similar equation for the (L.C.) gas. In these equations we suppress the superscript $(p+1)$ from T , τ , n , N , u , U and hence also from C , c , and F_0 . That is, at each step we take

8. Generally speaking, iteration is expected to be more rapidly convergent a procedure than successive approximations. In particular for the Boltzmann equation one must solve a non-linear integral equation at each step of an iteration procedure. On the other hand, in the Chapman-Enskog procedure, one is faced with a non-linear integral equation only at the initial step (when it is trivially solved) and at all other approximations one has a linear integral equation. The effect of the non-linearity is always thrown into the next approximation.

$$(4.2) \quad \int F^{(p+1)} \begin{bmatrix} 1 \\ \xi \\ \frac{M(\xi-U)^2}{2} \end{bmatrix} d\xi = \int F_0 \begin{bmatrix} 1 \\ \xi \\ \frac{M(\xi-U)^2}{2} \end{bmatrix} d\xi = \begin{bmatrix} N \\ NU \\ \frac{3}{2} NkT \end{bmatrix}$$

and these quantities change with the iterative step. The same relations and remarks apply to the (L.C.) gas. This guarantees the collision invariants (2.12,13), at each step of the procedure. Following the Chapman-Enskog procedure⁶, we shall remove temporal derivatives by means of the conservation equations as follows,

$$(4.3) \quad \left(\frac{\partial N}{\partial t}\right)^{p+1} = - \frac{\partial}{\partial x} (NU)$$

$$(4.4) \quad \left(\frac{\partial n}{\partial t}\right)^{p+1} = - \frac{\partial}{\partial x} (nu)$$

$$(4.5) \quad \left(\frac{\partial \tilde{u}}{\partial t}\right)^{p+1} = - \tilde{u} \cdot \frac{\partial}{\partial x} \tilde{u} + \frac{MN}{\tilde{\rho}} \mathcal{F} + \frac{mn}{\tilde{\rho}} f - \frac{1}{\tilde{\rho}} \frac{\partial \cdot P^{(p)}}{\partial x}$$

$$(4.6) \quad \left(\frac{\partial \tilde{e}}{\partial t}\right)^{p+1} = - \frac{\partial}{\partial x} \cdot \tilde{e} \tilde{u} - \frac{\partial}{\partial x} \cdot \tilde{Q}^{(p)} + \tilde{P}^{(p)} : \frac{\partial \tilde{u}}{\partial x} \\ + MN \mathcal{F} \cdot (u-U) + mn f \cdot (u-u) .$$

As before we suppress the superscript (p+1) from the "hydrodynamical" variables n, N, u, U, T, τ . In an obvious notation $\tilde{P}^{(n)}$ and $\tilde{Q}^{(n)}$ denote the stress and heat conduction (2.17) and (2.19) evaluated with $f^{(n)}, F^{(n)}$.

First Approximation

In the first approximation equation (4.1) becomes

$$(4.7) \quad 0 = \int (F_o - F^{(o)}) - \mu \frac{F_o(U-u) \cdot C}{NkT} - \frac{3vF_o}{2NkT} \left(\frac{C^2}{3RT} - 1 \right) (T-\tau) \\ + \mu_M \frac{F_o}{NkT} (U-u)^2 \left(\frac{C^2}{3RT} - 1 \right) ,$$

and similarly for the (L.C.) gas. It is immediately clear from the orthogonality relations of Hermite polynomials⁹ and relations (2.4,5) that (4.7) has the solution

$$(4.8) \quad u = U = \tilde{u}$$

$$(4.9) \quad T = \tau = \tilde{T}$$

$$(4.10) \quad \begin{cases} F_o = \tilde{F}_o \\ f_o = \tilde{f}_o . \end{cases}$$

This, of course, is in agreement with the Chapman-Enskog procedure which supplies at the initial step two local Maxwellians evaluated at mean conditions.

9. It is assumed that the reader is familiar with the properties of H. Grad's generalized Hermite polynomials. See H. Grad, Comm. Pure and Appl. Math. II, 325 (1949). An equivalent system of orthogonal polynomials in velocity space is given in terms of Sonine polynomials in reference 6.

Following the method given by equation (4.1) we now use (4.10) to give the second approximation.

Second Approximation

To carry out the second approximation we have to first calculate $D\tilde{f}_0$ and $D\tilde{F}_0$, and with the use of (4.3-6) eliminate time derivatives in these expressions. The calculation is straightforward and is readily found in the literature.¹⁰ On making these calculations the second approximation of the (U.C.) gas is given by

$$\begin{aligned}
 (4.11) \quad \tilde{F}_0 & \left[\frac{mn}{\tilde{\rho} \tilde{R} \tilde{T}} \tilde{C} \cdot (\mathcal{f} - \mathcal{F}) + \tilde{C} \cdot \frac{\partial \ell_n}{\partial x} \left(\frac{N}{\tilde{n}} \right) + \frac{n(m-M)}{\tilde{\rho}} C \cdot \frac{\partial}{\partial x} \ln \tilde{p} \right. \\
 & + \left(\frac{C_i C_j}{\tilde{R} \tilde{T}} - \delta_{ij} \right) \cdot \left(\frac{1}{2} \frac{\partial \tilde{u}_j}{\partial x_i} + \frac{1}{2} \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\delta_{ij}}{3} \frac{\partial u_k}{\partial x_k} \right) \\
 & \left. + \left(\frac{C^2}{2 \tilde{R} \tilde{T}} - \frac{5}{2} \right) \tilde{C} \cdot \frac{\partial}{\partial x} \ln \tilde{T} \right] \\
 & = \left[(F_0 - F) - \frac{\mu_{F_0}^F}{NkT} (U-u) \cdot C - \frac{\nu_{F_0}^F}{NkT} \left(\frac{C^2}{3 \tilde{R} \tilde{T}} - 1 \right) (T-\tau) \right. \\
 & \left. + \frac{\mu_{M_0}^F}{NkT} (U-u)^2 \left(\frac{C^2}{3 \tilde{R} \tilde{T}} - 1 \right) \right],
 \end{aligned}$$

with a similar equation for the (L.C.) gas. The superscript, indicating that this is the second approximation, has been

10. Chapter 8 of reference 6.

suppressed entirely since no higher approximations will be performed. One notices, in equation (4.11), two Maxwellians as opposed to just the mean Maxwellian which occurs in the Chapman-Enskog theory. This is due to the iteration scheme used above, as opposed to the successive approximations of Chapman-Enskog. Although this introduces more complexity into our calculations, it seems warranted by the latitude of the results. This will be seen in a moment.

Again using the orthogonality property of the polynomials, we obtain the following formulae from (4.11):

$$(4.12) \quad (u-U) = \frac{1}{\mu} \left[\frac{mnMn}{\tilde{\rho}} (\mathcal{f} - \mathcal{F}) + \frac{\tilde{n}k\tilde{T}}{2} \frac{\partial}{\partial x} \left(\frac{N-n}{\tilde{n}} \right) + \frac{nNkT(m-M)}{\tilde{\rho}} \frac{\partial}{\partial x} \ln \tilde{p} \right]$$

$$(4.13) \quad (T-\tau) = \frac{\mu\varepsilon}{v} \frac{Mm(N-n)}{\rho(M+m)} (U-u)^2 .$$

Before going on to the determination of stress and heat conduction, we pause to comment on (4.12,13). On comparing equation (4.12) with the diffusion expression given in Chapman and Cowling⁶, we notice that (4.12) does not contain thermal diffusion. It is shown in Appendix B that this is an exact result for molecules interacting with a Maxwell force law. For this and other reasons found in that appendix, equations (3.1,2) are models for a Maxwell gas. The extension of (3.1,2) to include thermal diffusion is not difficult and is given in

Appendix C. Next we note that in this approximation the Chapman-Enskog procedure predicts that the two gases are at the same temperature⁶ in contrast to (4.13). These two statements are easily brought into agreement. For in this approximation, inspection of the Chapman-Enskog procedure shows that quadratic collisional contributions are ignored and therefore (4.13) leads to $T \sim \tau$. On the other hand, it is shown in Appendix C that (4.13) is an exact result of iteration on the full Boltzmann equations.

From (4.11) and its (L.C.) counterpart we obtain the stress of the mixture to be,

$$(4.14) \quad \tilde{p}_{ij} = - \left(\frac{Nk\tilde{T}}{\Gamma} + \frac{nk\tilde{T}}{\gamma} \right) \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2\delta_{ij}}{3} \frac{\partial u_k}{\partial x_k} \right] \\ - \left[\frac{2mn\mu}{\tilde{\rho}\Gamma} + \frac{2MN\mu}{\tilde{\rho}\gamma} \right] \left[(U-u)_i(U-u)_j - \frac{(U-u)^2}{3} \delta_{ij} \right]$$

where \tilde{p}_{ij} is the divergenceless stress given by

$$(4.15) \quad p_{ij} = P_{ij} - \int \tilde{c}_i \tilde{c}_j (M\tilde{F}_0 + m\tilde{f}_0) d\xi .$$

On examining equation (4.14) we see that it contains a contribution due to velocity differences between the components of the gas. This is not generally included in the stress expression and again it is due to the iteration procedure. If, as before, we ignore quadratic velocity contributions to

force a correspondence with the method of successive approximations, we obtain precisely the same form for the stress as found in Chapman and Cowling.¹⁰

Finally we use (4.11) and the corresponding (L.C.) form to obtain the heat conduction relation:

$$(4.16) \quad Q = \frac{5}{2} k\tilde{T}[N(U-\tilde{u}) + n(U-\tilde{u})] - \frac{5}{2} k\tilde{T}\left(\frac{RN}{\bar{\Gamma}} + \frac{rn}{\gamma}\right)\frac{\partial\tilde{T}}{\partial x} + O[(u-U)^3]$$

where we have not explicitly given the $O([u-U]^3)$ term. The latter arises from the iterative part of the calculation which does not arise in the successive approximation procedure. Ignoring this latter term and comparing with the expression formed by means of the Chapman-Enskog procedure¹⁰, we see that (4.16) lacks a diffusion term. This should have been expected from the fact that (4.12) lacked a thermal diffusion component. In fact, as was pointed out before, our kinetic model is appropriate to a gas of Maxwell interaction, in which case the absence of diffusion in the heat conduction is an exact result, as is shown in Appendix B.

Our coefficients $\bar{\Gamma}$, γ , μ , ν , ϵ , which were left open, have by means of the transport theory given above, been associated with the heat conduction, viscosity, and diffusion coefficients. Therefore rather than obtain the former coefficients from kinetic theory, one may turn the tables and obtain the former coefficients from the latter.

Appendix A: Formal Derivation of the Binary Model Equations and Higher Approximations -- Linear Theory

This section is given in a somewhat perfunctory manner, since it is no more than a collage of techniques known in the literature. In particular we shall rely heavily on the techniques and notation developed by H. Grad^{7,11} and E. P. Gross and E. Jackson.¹²

It is our intention to give a formal procedure for developing kinetic models from an eigentheory basis, as was done in reference [12] for simple gases. Complexities attendant to gas mixtures restrict us and we avoid superfluous generality at the outset, and start with the restrictions which are ultimately forced upon us. (These are removed in Appendix C where a less formal procedure is employed.) More specifically, we consider gas mixtures for which all inter-particle effects are governed by a Maxwell force law. Further, we linearize about mean (but local) Maxwellians. With these restrictions the cross-collision integrals may be represented by

$$\begin{aligned}
 (A.1) \quad J(f, F) &\sim \mathcal{L}_f(g) + \mathcal{L}_F(G) \\
 &= \int \tilde{f}_o \tilde{F}_{o1} [G(\xi'_1) - G(\xi_1)] B(\theta) d\varepsilon d\theta d\xi_1 \\
 &\quad + \int \tilde{f}_o \tilde{F}_{o1} [g(\xi'_1) - g(\xi)] B(\theta) d\varepsilon d\theta d\xi_1
 \end{aligned}$$

11. H. Grad, "Principles of the Kinetic Theory of Gases", in Handbuch der Physik, vol. 12 (Springer, 1958).

12. E. P. Gross and E. Jackson, Phys. Fluids 2, 432 (1959).

and a similar relation for the (U.C.) cross-collision term.

In (A.1) we have taken

$$(A.2) \quad F = \tilde{F}_0(1 + G)$$

$$(A.3) \quad f = \tilde{f}_0(1 + g)$$

In the notation of Section 2 we write

$$(A.4) \quad V = (\xi - \tilde{u})/\sqrt{R\tilde{T}}$$

$$(A.5) \quad v = (\xi - \tilde{u})/\sqrt{r\tilde{t}}$$

and expand the distribution functions in Hermite polynomials¹¹,

$$(A.6) \quad F = \tilde{F}_0 \left[1 + \sum_{k=1}^{\infty} \frac{A_i^{(k)}(x, t) H_i^{(k)}(V)}{k!} \right]; \quad A_i^{(k)} = \frac{1}{MN} \int F H_i^{(k)} d\xi$$

$$(A.7) \quad f = \tilde{f}_0 \left[1 + \sum_{k=1}^{\infty} \frac{a_i^{(k)}(x, t) H_i^{(k)}(v)}{k!} \right]; \quad a_i^{(k)} = \frac{1}{mn} \int f H_i^{(k)} d\xi.$$

We also expand the integral operators $\mathcal{L}_f(g)$ and $\mathcal{L}_f(G)$ in Hermite polynomials

$$(A.8) \quad \mathcal{L}_f(G) = \tilde{f}_0 \sum_{\substack{k, \ell \\ k \neq 0}}^{\infty} \frac{A_i^{(k)} B_{ij}^{(k\ell)} H_j^{(\ell)}(v)}{k! \ell!}$$

$$(A.9) \quad \mathcal{L}_f(g) = \tilde{f}_0 \sum_{k, \ell}^{\infty} \frac{a_i^{(k)} \beta_{ij}^{(k\ell)} H_j^{(\ell)}(v)}{k! \ell!} .$$

The form of equation (A.1) clearly dictates that the latter expansions be taken about \tilde{f}_0 rather than \tilde{F}_0 . On the other hand, in analyzing $J(F, f)$ just the contrary is true.

A straightforward calculation yields,

$$(A.10) \quad \beta_{ij}^{(k\ell)} = \frac{Nn}{(2\pi)^3} \int e^{-\frac{V_1^2 + v^2}{2}} dv dV_1 B(\theta) d\theta d\varepsilon H^{(\ell)}(v) [H_i^{(k)}(v') - H_i^{(k)}(v)]$$

$$(A.11) \quad B_{ij}^{(k\ell)} = \frac{Nn}{(2\pi)^3} \int e^{-\frac{V_1^2 + v^2}{2}} dv dV_1 B(\theta) d\theta d\varepsilon H_j^{(\ell)}(v) [H_i^{(k)}(V_1') - H_i^{(k)}(V_1)] .$$

These are the tensorial forms of the usual "bracket integrals". We now show, by an argument first given by Grad³, that the last two expressions are zero unless $k = \ell$. The θ -integration of the bracket in (I.10,11) results in a polynomial of order k , and so by the orthogonality of the Hermite polynomials (I.10,11) vanish unless $k \geq \ell$. Next, since $dv dV_1 = dv d'V_1'$ and $v^2 + V_1^2 = v'^2 + V_1'^2$ the argument is reversed. We can, therefore, now write,

$$(A.12) \quad \mathcal{L}_f(G) = \tilde{f}_0 \sum_{k=1}^{\infty} \frac{A_i^{(k)} B_{ij}^{(k)} H_j^k}{k!k!}$$

$$(A.13) \quad \mathcal{L}_f(g) = \tilde{f}_0 \sum_{k=1}^{\infty} \frac{a_i^{(k)} \beta_{ij}^{(k)} H_j^k}{k!k!} .$$

Following Grad¹³ we introduce contracted tensors, and then from the isotropy of the integral operator we may write

$$(A.14) \quad \mathcal{L}_f(G) = \tilde{f}_0 \sum_{\substack{k=1 \\ m}}^{\infty} \frac{A_i^{(k,m)} B^{(k,m)} H_i^{(k,m)}(v)}{k!}$$

$$(A.15) \quad \mathcal{L}_f(g) = \tilde{f}_0 \sum_{\substack{k=1 \\ m}}^{\infty} \frac{a_i^{(k,m)} \beta^{(k,m)} H_i^{(k,m)}(v)}{k!}$$

where the $B^{(k,m)}$ and $\beta^{(k,m)}$ are proportional to "cross-sections" and are in fact eigenvalues for the problem. We have in fact shown,

$$(A.16) \quad \mathcal{L}_f(H_i^{(k,m)}(v)) = \tilde{f}_0 \beta^{(k,m)} H_i^{(k,m)}(v)$$

$$(A.17) \quad \mathcal{L}_f(H_i^{(k,m)}(v)) = f_0 \beta^{(k,m)} H_i^{(k,m)}(v) .$$

We see from (A.16) that the $H^{(k,m)}(v)$ are eigenfunctions and the $\beta^{(k,m)}$ eigenvalues of \mathcal{L}_f . On the other hand, from (A.17)

13. Section 30 of reference 11.

the $H^{(k,m)}(V)$ are not, strictly speaking, eigenfunctions although we shall, in a broader sense, refer to them as such. The pseudo-eigenfunction property (A.17) is in fact more valuable to us since it furnishes us with only one type of eigenfunction in any single Boltzmann equation.

In the more familiar notation of Sonine polynomials and Legendre polynomials¹², we can rewrite (A.16) and (A.17) as

$$(A.18) \quad \mathcal{I}_f[S_{\ell+\frac{1}{2}}^r (v^2/2)v^\ell P_\ell^m(\cos \psi)e^{im\phi}]$$

$$= \tilde{f}_o \lambda_{r\ell} S_{\ell+\frac{1}{2}}^r (v^2/2)v^\ell P_\ell^m(\cos \psi)e^{im\phi}$$

$$(A.19) \quad \mathcal{I}_f[S_{\ell+\frac{1}{2}}^r (v^2/2)v^\ell P_\ell^m(\cos \psi)e^{im\phi}]$$

$$= \tilde{f}_o \Lambda_{r\ell} S_{\ell+\frac{1}{2}}^r (v^2/2)v^\ell P_\ell^m(\cos \psi)e^{im\phi}$$

C. F. Curtiss¹⁴, in considering the relaxation theory of an isotropic ($\ell = m = 0$) Maxwellian gas mixture showed many of the above properties and computed the Λ and λ for $\ell = 0$.

Following the work of Gross and Jackson¹², we can now easily develop a formal procedure for obtaining model equations. Again we mention that, although our calculations are for a two-component mixture, the generalization to a multi-component mixture is trivial. Introducing an ordering to the eigenfunctions

14. C. F. Curtiss, "The Rate of Equilibration of Translational Kinetic Energy in Gas Mixtures", Univ. of Wisc., Dept. of Chem., NSF-2746 (1957).

and denoting them simply by ϕ_n , we write

$$(A.20) \quad Df = \tilde{f}_0 \sum a_n \lambda_n \phi_n(v) + f_0 \sum a_n \lambda_n^f \phi_n(v) \\ + \sum A_n \lambda_n^F \phi_n(v),$$

$$(A.21) \quad DF = \tilde{F}_0 \sum A_n \Lambda_n \phi_n(v) + \tilde{F}_0 \sum A_n \Lambda_n^F \phi_n(v) \\ + \sum a_n \Lambda_n^f \phi_n(v) ,$$

where the first series of the right hand side gives the self-collision effect¹⁵ and the remaining two, the cross-collision effect. A relaxation analysis of this system¹⁴, shows that a_n , A_n can be considered in pairs, and that all but the lowest coefficients (density, temperature, velocity) vanish exponentially. With this in mind, we take as the N^{th} order model equations,

$$(A.22) \quad Df = \tilde{f}_0 \sum_{n=1}^N a_n \lambda_n \phi_n(v) - \gamma_N \tilde{f}_0 \sum_{n=N+1}^{\infty} a_n \phi_n(v) \\ + \tilde{f}_0 \sum_{n=1}^N a_n \lambda_n^f \phi_n(v) + \tilde{f}_0 \sum_{n=1}^N A_n \lambda_n^F \phi_n(v) \\ = \gamma_N (f_0 - f) + \tilde{f}_0 \sum_{n=1}^N a_n (\lambda_n + \gamma_N) \phi_n(v) \\ + \tilde{f}_0 \sum_{n=1}^N a_n \lambda_n^f \phi_n(v) + f_0 \sum_{n=1}^N A_n \lambda_n^F \phi(v),$$

15. The self-collision analysis was first given by C. S. Wang Chang and G. E. Uhlenbeck in "On the Propagation of Sound in a Monatomic Gas," Univ. of Mich. Engr. Rep. (1954). Our analysis parallels the treatment of Grad in reference 11.

$$\begin{aligned}
(A.23) \quad DF = \Gamma_n(\tilde{F}_0 - F) + \tilde{F}_0 \sum_{n=1}^N A_n(\Lambda_n + \Gamma_n)\phi_n(V) \\
+ \tilde{F}_0 \sum_{n=1}^N A_n \Lambda_n^F \phi_n(V) + \tilde{F}_0 \sum_{n=1}^N a_n \Lambda_n^f \phi_n(V) .
\end{aligned}$$

In equation (I.22) we have indicated the device used by Gross and Jackson.¹⁶ A relaxation theory of (A.22,23) clearly shows that they accurately preserve the relaxation theory of (A.20, 21) for all coefficients up to and including the coefficients a_n and A_n . For all other moments the relaxation theory is qualitatively preserved in as much as an exponential decay of all higher coefficients is predicted. The a_n ($n > N$) have a decay time of $1/\gamma_N$ and the A_n ($n > N$) a decay time of $1/\Gamma_N$.

The γ_N , Γ_N and the coefficients a_n , A_n for $n \leq N$, must be artfully chosen. A discussion of this would be superfluous since the same considerations as found in the literature of simple gases¹⁷, also apply here.

One notices that the second and third summations of (A.22,23) may be combined. This should not be hastily done, since in practice it turns out convenient to split the third summation between the last and second summations. This is indicated below.

16. This is given in reference 12. An extension of their technique is given in Appendix D.

17. See reference 12. A slight improvement of this technique is to be found in the following report by the author: "The Initial Value Problem, Sound Propagation, and Modeling in Kinetic Theory", AFOSR-1380, Courant Institute of Math. Sci., NYU (1961).

As an example of the above procedure we carry out some of the details for the case comparable to Sections 2 and 3. The expansion of the distribution functions about mean Maxwellians leads to,

$$(A.24) \quad F = \tilde{F}_0 \left\{ 1 + \frac{(U-\tilde{u})}{\sqrt{R\tilde{T}}} \cdot v + \frac{3}{2} \frac{(T-\tilde{T})}{\tilde{T}} \left(\frac{v^2}{3} - 1 \right) + O[(U-u)^2, \dots] \right\}$$

$$(A.25) \quad f = \tilde{f}_0 \left\{ 1 + \frac{(u-\tilde{u})}{\sqrt{R\tilde{T}}} \cdot u + \frac{3}{2} \frac{(\tau-\tilde{T})}{\tilde{T}} \left(\frac{v^2}{3} - 1 \right) + O[(u-\tilde{u})^2, \dots] \right\}.$$

When substituted into the cross-collision operators these become

$$(A.26) \quad \mathcal{L}_F(g) + \mathcal{L}_F(G) = \tilde{f}_0 \left[\frac{\lambda(u-U)}{\sqrt{r\tilde{T}}} \cdot v + \frac{3}{2} \Lambda \frac{(\tau-T)}{\tilde{T}} \left(\frac{v^2}{3} - 1 \right) + \dots \right]$$

$$(A.27) \quad \mathcal{L}_F(g) + \mathcal{L}_F(G) = \tilde{F}_0 \left[\frac{mn}{MN} \frac{\lambda(U-u)}{\sqrt{R\tilde{T}}} \cdot v + \frac{3}{2} \frac{n\Lambda}{N} \frac{(T-\tau)}{\tilde{T}} \left(\frac{v^2}{3} - 1 \right) + \dots \right].$$

We have neglected quadratic deviations from the mean flow since terms of this order have already been neglected in linearizing the collision integral. The values of λ and Λ are not difficult to compute and are given by

$$(A.28) \quad \lambda = 2NA_1 \left(\frac{mM}{M+m} \right)^{1/2} \pi \sqrt{2\kappa}$$

$$(A.29) \quad \Lambda = 2\lambda.$$

In this κ is the proportionality constant in the inter-

molecular force law and A_1 is a cross-section whose numerical value is given by,¹⁸

$$(A.30) \quad A_1 = .422.$$

Referring to equations (A.22,23) the model equations under consideration are

$$(A.31) \quad D\tilde{f} = \gamma \left[\tilde{f}_o \left\{ 1 + \frac{(u-\tilde{u})}{\sqrt{r\tilde{T}}} \cdot v + \frac{3}{2} \frac{(\tau-\tilde{T})}{\tilde{T}} \left(\frac{v^2}{3} - 1 \right) \right\} - f \right] \\ + \tilde{f}_o \left[\frac{\lambda(u-U)}{\sqrt{r\tilde{T}}} \cdot v + \frac{3}{2} \Lambda \frac{(\tau-T)}{\tilde{T}} \left(\frac{v^2}{3} - 1 \right) \right]$$

$$(A.32) \quad DF = \Gamma \left[\tilde{F}_o \left\{ 1 + \frac{(U-\tilde{u})}{\sqrt{R\tilde{T}}} \cdot v + \frac{3}{2} \frac{(T-\tilde{T})}{\tilde{T}} \left(\frac{v^2}{3} - 1 \right) \right\} - F \right] \\ + F_o \left[\frac{mn}{MN} \lambda \frac{(U-\tilde{u})}{\sqrt{R\tilde{T}}} \cdot v + \frac{3}{2} \frac{n\Lambda}{N} \frac{(T-\tau)}{\tilde{T}} \left(\frac{v^2}{3} - 1 \right) \right] .$$

It should be noted that the first bracket of each of the above equations is the linearization about a mean Maxwellian of the deviation from a local Maxwellian, which is found for the simple gas treatment. Alternately, equations (A.31,32) are the mean linearized forms of (3.1,2) which were postulated. As mentioned earlier, the γ and Γ should be chosen to fulfill some particular purpose. Finally, Λ and λ need not be chosen according to (A.28,29) since the conservation laws will be satisfied independent of their choice.

18. Ref. 6, page 173.

Appendix B: Maxwell Force Modeling

We may represent equations (2.9) and (2.10) as follows:

$$(B.1) \quad Df = J(f, f) + J(f, F)$$

$$(B.2) \quad DF = J(F, F) + J(F, f).$$

Again distinguishing between a successive approximation scheme and an iteration procedure, the iteration on (B.1,2) is given by

$$(B.3) \quad Df^{(n-1)} = J(f^{(n)}, f^{(n)}) + J(f^{(n)}, F^{(n)})$$

$$(B.4) \quad DF^{(n-1)} = J(F^{(n)}, F^{(n)}) + J(F^{(n)}, f^{(n)}) .$$

As is shown in reference 6 (Section 4.3), the solution to the first approximation is given by (2.2) and (2.3), i.e.,

$$(B.5) \quad f^{(0)} = \tilde{f}_0$$

$$(B.6) \quad F^{(0)} = \tilde{F}_0 .$$

The second approximation is then obtained from

$$(B.7) \quad D\tilde{f}_0 = J(f^{(1)}, f^{(1)}) + J(f^{(1)}, F^{(1)})$$

$$(B.8) \quad D\tilde{F}_0 = J(F^{(1)}, F^{(1)}) + J(F^{(1)}, f^{(1)}) ,$$

where the left hand sides have been already calculated in

(4.11). We now compute the following two integrals:

$$(B.9) \quad A = \int \xi J(f, F) d\xi$$

$$(B.10) \quad B = \int (\xi - \tilde{u})^2 J(f, F) d\xi$$

for particles interacting with a Maxwell force law. In this case we have

$$(B.11) \quad A = \int \xi \int [F(\xi'_1) f(\xi') - F(\xi_1) f(\xi)] B(\theta) d\epsilon d\theta d\xi_1 d\xi$$

$$= \iint (\xi' - \xi) B(\theta) d\epsilon d\theta F(\xi_1) f(\xi) d\xi_1 d\xi.$$

The last step makes use of a well-known integral relationship.¹⁹ Note that in a two-particle collision

$$(B.12) \quad \xi' - \xi + \frac{2M}{m+M} (\xi_1 - \xi) \cdot \alpha \alpha$$

where α orients a collision²⁰ ($\alpha = \alpha(\theta, \epsilon)$). From the isotropy of space

$$(B.13) \quad \int (\xi' - \xi) B(\theta, \epsilon) d\epsilon d\theta \sim (\xi_1 - \xi).$$

The proportionality constant (a cross-section) is immaterial to us for the moment. Substitution into (B.11) therefore shows

19. Reference 6, page 67.

20. Reference 9, page 387.

$$(B.14) \quad A = a(U-u).$$

A similar argument shows us

$$(B.15) \quad B = b_1(T-\tau) + b_2(U-u)^2.$$

The proportionality factors are functions of density and temperature which will be given shortly. Referring to (B.7,8) we have, therefore, shown that relations (4.12) and (4.13) are exact for Maxwell molecules. In particular, the absence of thermal diffusion is exact for molecules interacting with a Maxwell potential.

The proportionality factors which occur in equations (B.14) and (B.15) above may be obtained from the calculations of I. Kolodner²¹, and they are

$$(B.16) \quad a = - \frac{\lambda}{m}$$

$$(B.17) \quad b_1 = - \frac{6k}{M} \lambda$$

$$(B.18) \quad b_2 = - \frac{2}{M} \frac{(n-N)}{m+M} \frac{Mm}{\rho} \lambda$$

where

$$(B.19) \quad \lambda = A_1 2\pi nN \left(\frac{2\kappa Mm}{M+m} \right)^{1/2}.$$

Here κ is the intermolecular force law constant, k is

21. I. Kolodner, "Moment Description of Gas Mixtures I", NYO-7980, Inst. of Math. Sci., NYU (1957).

Boltzmann's constant, and A_1 is a cross-section, the numerical value of which is given by (A.30).

The discussion of this section provides another basis for the equations postulated in Section 3. The work of Section 4 gave a presumably asymptotic technique for describing a gaseous mixture. If one examines the results obtained, one sees that the description of the gas mixture is in terms of a single fluid, the mean fluid. By this is meant that only one continuity, momentum, and energy equation enters into the resulting theory. Another macroscopic theory which provides much more detail is one for which one continuity, momentum, and energy equation is given for each gas component. For a Maxwell force interaction the postulated equations give the same collision term contribution as the exact theory. Another way of stating it is that the mass, momentum, and energy moments of the postulated equations for each species is identical to those of the Boltzmann equations for a Maxwell interacting gas.

Appendix C: Non-linear, Non-Maxwell Modeling

Before going on to our discussion it should be noted that for us the use of the word "linear" only refers to the collision integral. It is in fact the case that the linearized

analysis of the previous section leads to a non-linear theory. Linearization only refers to whether the distribution function occurs explicitly in a linear way.

The formalism which led to the model equations of the last section was fashioned after the work of Gross and Jackson. No rigorous basis exists for this formalism although the elegance of the procedure does promote some confidence. We now remove the restriction of Maxwell molecules and linearity and give a general formal procedure for obtaining kinetic models. Although the procedure is less elegant than that given by Gross and Jackson¹², it reduces to theirs under linearization and the imposition of a Maxwell force law.

We first consider a simple gas. The Boltzmann equation is represented by

$$(C.1) \quad Df = J(f,f) \quad .$$

The collision integral may be expanded in Hermite polynomials²² to give

$$(C.2) \quad J(f,f) = \frac{\rho f_0}{2} \sum_{n=2}^{\infty} \sum_{r,s=0}^{\infty} \frac{\beta_{ijk}^{(nrs)} H_i^{(n)} a_j^{(r)} a_k^{(s)}}{n!}$$

22. Reference 11, Section 28.

$$(C.3) \quad \beta_{ijk}^{(nrs)} = \frac{1}{r!s!} \int \frac{1}{m} B(\theta, |\xi_1 - \xi|) e^{\frac{v^2 + v_1^2}{2}} H_j^{(r)}(v) H_k^s(v_1) [H_i^{(n)}] d\epsilon d\theta dv_1 dv$$

with

$$[\phi] = \phi'_1 + \phi' - \phi_1 - \phi.$$

We approximate the collision integral simply by

$$(C.4) \quad J^N(f, f) = \frac{\rho f_o}{2} \sum_{n=2}^N \sum_{r,s=0}^N \frac{\beta_{ijk}^{(nrs)} H_i^{(n)} a_j^{(r)} a_k^{(s)}}{n!}$$

$$= v_N \rho f_o \sum_{n=N+1}^{\infty} \frac{a_i^{(n)} H_i^{(n)}}{n!}$$

$$= v_N \rho (f_o - f) + \frac{\rho_o f_o}{2} \sum_{n=2}^N \sum_{r,s=0}^N \frac{\hat{\beta}_{ijk}^{(nrs)} H_i^{(n)} a_j^{(r)} a_k^{(s)}}{n!}$$

where

$$(C.5) \quad \hat{\beta}_{ik}^{(nno)} = \hat{\beta}_{ik}^{(non)} = \beta_{ik}^{(non)} - v_N \delta_{ik}^n, \quad \delta_{ik}^n = \delta_{i_1 k_1} \delta_{i_2 k_2} \dots \delta_{i_n k_n},$$

and for all other β 's

$$(C.6) \quad \hat{\beta}_{ijk}^{(nrs)} = \beta_{ijk}^{(nrs)}.$$

It is clear that a specialization to Maxwell molecules ($n = r + s$) and a linearization (either $r = 0$, or $s = 0$) reduces the approximation of (C.4) to that previously given. Further, it accurately gives a certain "block" of coefficients and approximates the high moments of the distribution by exponential decay in a relaxation theory.

The extension to mixtures is quite clear. Self-collisions are treated as above while the series expansions for cross-collision integrals are merely terminated as in Appendix A. A major consideration now lies in the choice of a Maxwellian to expand about. This is of crucial importance in the evaluation of collisional integrals. In a paper containing many important calculations, I. Kolodner²¹ computed many collisional integrals for the cross-collision term. He expands in Maxwellians with mean velocity but component temperatures. All constants necessary for a "13-moments" description are given by Kolodner. That is, the summation corresponding to that of (C.4) contains the stress and heat conduction. Kolodner points out that the expansion about component Maxwellians (which, of course, would be more flexible) leads to formidable computational difficulties.

It is no doubt the case that insofar as problem solving is concerned, the kinetic models just given above allow no more penetration than do the full Boltzmann equations. On the other hand such kinetic models greatly simplify the Chapman-Enskog procedure. For instance, a "13 moments" model contains more

than enough detail to furnish the complete Navier-Stokes²³ and Burnett equations. In another area it should be much simpler to show existence and uniqueness for the non-linear models than for the non-linear Boltzmann equation. This perhaps could be used as a basis for dealing with the latter problem.

Appendix D: Collision Integral Approximation.

In this section we generalize the cut-off device of Gross and Jackson which was used earlier. Again it is only necessary to consider a simple gas. We consider the linearized Boltzmann equation and denote the collision operator by \mathcal{L} and the eigenvalues and eigenfunctions by $\lambda_n, \{\phi_n\}$ respectively.

We have

$$(D.1) \quad f = f_0(1 + g) = f_0 \left(1 + \sum_{n=1}^{\infty} a_n \phi_n \right)$$

$$(D.2) \quad J(f, f) \sim \mathcal{L}(f_0 g) = f_0 \sum a_n \lambda_n \phi_n$$

that is,

$$(D.3) \quad \mathcal{L}(f_0 \phi_n) = \lambda_n \phi_n f_0 .$$

23. In fact, only the local linearization of the "13 moments" description is necessary for the Navier-Stokes theory.

Suppose we have another operator L such that it too has $\{\phi_n\}$ as eigenfunctions, i.e.,

$$(D.4) \quad L(\phi_n) = \mu_n \phi_n$$

We approximate \mathcal{L} to the N^{th} order by means of L as follows:

$$(D.5) \quad \begin{aligned} \mathcal{L}(g) &\approx f_0 \sum_{n=0}^N a_n \lambda_n \phi_n + \lambda^N f_0 \sum_{n=N+1}^{\infty} a_n \mu_n \phi_n \\ &= f_0 \sum_{n=0}^{\infty} a_n (\lambda_n - \lambda^N \mu_n) \phi_n + \lambda^N L(f_0 g) . \end{aligned}$$

The only essential requirement on L is that for n large it be negative, i.e.,

$$(D.6) \quad (\phi_n, L\phi_n) < 0.$$

It goes without saying that approximating \mathcal{L} by L is valueless unless L is more tractable than \mathcal{L} . Again the λ^N is to be judiciously chosen.

The equations of Gross and Jackson are obtained by taking L to be the constant operator, i.e.,

$$(D.7) \quad L(\phi_n) = v \phi_n$$

where v is independent of n . This introduces an infinite degeneracy which imposes a series limitation on the equation.¹⁹

For Maxwell molecules (the only case for which the eigenfunctions are known) another operator is available to us. It is shown in a paper by Lebowitz, Frisch, and Helfand²⁴ that

$$(D.8) \quad L = \frac{\partial}{\partial \xi_j} [(\xi - u)_j + \frac{kT}{m} \frac{\partial}{\partial \xi_j}] f_0 H_i^{(k)}(v) = -k f_0 H_i^{(k)}(v)$$

where k is an integer corresponding to the order of the Hermite polynomial $H_i^{(k)}$. It will be recalled that the correct eigenfunctions are the contracted Hermite polynomials $H_i^{(m,n)}(v)$, hence the operator of (D.8) introduces a degeneracy among eigenfunctions of the same degree. Using this operator approximation the equation corresponding to the simplest cut-off is

$$(D.9) \quad Df = v \frac{\partial}{\partial \xi} \cdot [(\xi - u) + \frac{kT}{m} \frac{\partial}{\partial \xi}] f.$$

This is the equation considered in reference 24.

It was shown by Mott-Smith²⁵ that the eigenvalues for Maxwell grow as the fourth root of the degree of the corresponding Hermite polynomial. From this fact we see that the single relaxation model over-estimates the role of the higher moments of the distribution function, whereas the model given by (D.10) underestimates the effect of the higher moments.

24. J. L. Lebowitz, H. L. Frisch, and E. Helfand, Phys. of Fluids 3, 325 (1960).

25. H. M. Mott-Smith, "A New Approach to the Kinetic Theory of Gases", Lincoln Laboratory, MIT (1954).

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